2-METHYLHEXANEDIOIC ACID

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 52.6 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.29e-01

Confidence level: 7.17e-01

Nearest Neighbors from the Training Set

Image not found
N-Methyl-N'-phenylurea
Measured: 19.5
Predicted: 29.8

Image not found
Urea, (3-methylphenyl)-
Measured: 36.3
Predicted: 37.2

Image not found
Metaldehyde acetaldehyde tetramer
Measured: 240
Predicted: 148

Image not found
Urea, 1-(p-fluorophenyl)-
Measured: 33.1
Predicted: 49.6

Image not found
N-(3-chlorophenyl)-N'-methylurea
Measured: 85.1
Predicted: 101